Contents

Conference Photograph vi
Foreword and Acknowledgments vii
Conference Information viii
Sponsors x

Closing remarks

To 40 years of defects in semiconductors: may the problem never be solved!
M. Stavola 1

1. Plenary

Self-interstitials in semiconductors: what we are learning from interstitial Zn in ZnSe
G.D. Watkins and K.H. Chow 7

Current problems in diamond: towards a quantitative understanding
G. Davies 15

The role of threading dislocations in the physical properties of GaN and its alloys
J.S. Speck and S.J. Rosner 24

2. Gallium nitride

2.1. Doping

Observation of Ga vacancies and negative ions in undoped and Mg-doped GaN bulk crystals
K. Saarinen, J. Nissilä, J. Oila, V. Ranki, M. Hakala, M.J. Puska, P. Hautojärvi, J. Likonen, T. Suski, I. Grzegory, B. Lucznik and S. Porowski 33

Mechanism of radiative recombination in acceptor-doped bulk GaN crystals
M. Godlewski, T. Suski, I. Grzegory, S. Porowski, J.P. Bergman, W.M. Chen and B. Monemar 39

Mg acceptors in GaN: Dependence of the g-anisotropy on the doping concentration
D.M. Hofmann, W. Burkhardt, F. Leiter, W. von Förster, H. Alves, A. Hofstaetter, B.K. Meyer, N.G. Romanov, H. Amano and I. Akasaki 43

Electrical characterization of Mg-related energy levels and the compensation mechanism in GaN : Mg
D. Seghier and H.P. Gislason 46

Effect of Si doping on the strain and defect structure of GaN thin films
L.T. Romano, C.G. Van de Walle, B.S. Krusor, R. Lau, J. Ho, T. Schmidt, J.W. Ager III, W. Götz and R.S. Kern 50

Photo-enhanced dissociation of hydrogen-magnesium complexes in gallium nitride
Y. Kamiura, Y. Yamashita and S. Nakamura 54

Optically detected magnetic resonance of shallow donor – shallow acceptor and deep (2.8–3.2 eV) recombination from Mg-doped GaN
E.R. Glaser, T.A. Kennedy, J.A. Freitas Jr., B.V. Shanabrook, A.E. Wickenden, D.D. Koleske, R.L. Henry and H. Obloh 58

The role of deep levels in the persistent photoconductivity in Mg-doped GaN grown by MOCVD
D. Seghier and H.P. Gislason 63

High-resolution PL spectra of donor- and acceptor-bound excitons in homoepitaxial GaN-layers
K. Kornitzer, M. Grehl, K. Thonke, R. Sauer, C. Kirchner, V. Schwegler, M. Kamp, M. Leszczynski, I. Grzegory and S. Porowski 66

2.2. Point defects

Defect formation near GaN surfaces and interfaces
L.J. Brillson, T.M. Levin, G.H. Jessen, A.P. Young, C. Tu, Y. Naoi, F.A. Ponce, Y. Yang, G.J. Lapeyre, J.D. MacKenzie and C.R. Abernathy 70

Selective excitation of the yellow luminescence of GaN
J.S. Colton, P.Y. Yu, K.L. Teo, P. Perlin, E.R. Weber, I. Grzegory and K. Uchida 75

Transient photoluminescence of defects in undoped GaN prepared by metal organic vapor phase epitaxy
R.Y. Korotkov, M.A. Reshchikov and B.W. Wessels 80

Defect introduction in epitaxially grown n-GAN during electron beam deposition of Ru schottky contacts
F.D. Auret, S.A. Goodman, G. Myburg, F.K. Koschnick, J.-M. Spaeth, B. Beaumont and P. Gibart 84

Influence of generalized gradient approximations on theoretical hyperfine fields of paramagnetic defects
U. Gerstmann and H. Overhof 88

Metastable-like behaviour of a sputter deposition-induced electron trap in n-GaN
F.D. Auret, W.E. Meyer, S.A. Goodman, F.K. Koschnick, J.-M. Spaeth, B. Beaumont and P. Gibart 92

Annealing of ion-implanted GaN
A. Burchard, E.E. Haller, A. Stötzler, R. Weissenborn, M. Deicher and ISOLDE Collaboration 96

Behavior of electrically active point defects in irradiated MOCVD n-GaN
V.V. Emtsev, V.Yu. Davydov, V.V. Kozlovskii, D.S. Poloskin, A.N. Smirnov, N.M. Shmidt and A.S. Usikov 101

2.3. Impurities

Deep acceptors in undoped GaN
M.A. Reshchikov, F. Shahedipour, R.Y. Korotkov, M.P. Ulmer and B.W. Wessels 105

Correlation of vibrational modes and DX-like centers in GaN:O
C. Wetzel, J.W. Ager III, M. Topf, B.K. Meyer, H. Amano and I. Akasaki 109

Effects of oxygen incorporation in p-type AlN crystals doped with carbon species
T. Yamamoto and H. Katayama-Yoshida 113

Negatively charged muonium states in gallium nitride
R.L. Lichti, M.R. Dawdy, T.L. Head, S.F.J. Cox, B. Hitti and C. Schwab 116

ODMR of bound excitons in Mg-doped GaN
M.W. Bayerl, M.S. Brandt, T. Suski, I. Grzegory, S. Porowski and M. Stutzmann 120

2.4. Extended defects

Ordering in bulk GaN : Mg samples: defects caused by Mg doping
Z. Liliental-Weber, M. Benamara, W. Swider, J. Washburn, I. Grzegory, S. Porowski, R.D. Dupuis and C.J. Eiting 124

Structure of the $\{1\,1\,\underline{2}\,0\}$ inversion domain boundary in GaN
J.E. Northrup 130

Electronically induced dislocation glide motion in hexagonal GaN single crystals
K. Maeda, K. Suzuki, M. Ichihara, S. Nishiguchi, K. Ono, Y. Mera and S. Takeuchi 134

Role of the defect microstructure on the electrical transport properties in undoped and Si-doped GaN grown by LP-MOVPE
J.-L. Farvacque, Z. Bougrioua, I. Moerman, G. Van Tendeloo and O. Lebedev 140

Identification of Ag and Cd photoluminescence in ^{111}Ag-doped GaN
A. Stötzler, R. Weissenborn and M. Deicher 144

Cathodoluminescence intensity and dislocation contrast evolutions under electron beam excitation in epitaxial GaN laterally overgrown on (0 0 0 1) sapphire
S. Dassonneville, A. Amokrane, B. Sieber, J.-L. Farvacque, B. Beaumont, V. Bousquet, P. Gibart, K. Leifer and J.-D. Ganiere 148

3. Silicon

3.1. Hydrogen

Spectroscopic studies of H-decorated interstitials and vacancies in thin-film silicon exfoliation
Y.J. Chabal, M.K. Weldon, Y. Caudano, B.B. Stefanov and K. Raghavachari 152

The dipole moments of H_2, HD and D_2 molecules and their concentrations in silicon
R.C. Newman, R.E. Pritchard, J.H. Tucker and E.C. Lightowlers 164

Deep levels of vacancy-hydrogen centers in silicon studied by Laplace DLTS
K.B. Nielsen, L. Dobaczewski, K. Goscinski, R. Bendesen, O. Andersen and B.B. Nielsen 167

Hydrogen-induced extended complexes in silicon
Yu.V. Gorelkinskii, Kh.A. Abdullin and B.N. Mukashev 171

Optically active hydrogen dimers in silicon
B. Hourahine, R. Jones, A.N. Safonov, S. Öberg, P.R. Briddon and S.K. Estreicher 176

The *A* center binding a single hydrogen atom in crystalline silicon observed by EPR
P. Johannesen, J.R. Byberg and B. Bech Nielsen 180

Effects of charge state on stress-induced alignment and relaxation of a hydrogen–carbon complex in silicon
K. Fukuda, Y. Kamiura and Y. Yamashita 184

A new type of hydrogen molecules in silicon
K. Murakami, K. Ishioka, M. Kitajima, S. Tateishi, K. Nakanoya, T. Mori and S. Hishita 188

Temperature dependence of the formation of hydrogen molecules in n- and p-type silicon
M. Kitajima, K. Ishioka, K. Murakami, K. Nakanoya and T. Mori 192

Vibration of hydrogen molecules in semiconductors: anharmonicity and electron correlation
M. Saito, Y. Okamoto, A. Oshiyama and T. Akiyama 196

Microscopic properties of H_2 in Si from the dependence of the 3618.4 cm^{-1} line on temperature and stress
J.A. Zhou, E. Chen and M. Stavola 200

Hydrogen interactions with interstitial- and vacancy-type defects in silicon
S.Zh. Tokmoldin, B.N. Mukashev, Kh.A. Abdullin and Yu.V. Gorelkinskii 204

Vacancy–hydrogen complexes in group-IV semiconductors
M. Budde, B.B. Nielsen, J.C. Keay and L.C. Feldman 208

Nucleation mechanism of hydrogen-induced platelets in single crystal and polycrystalline silicon
N.H. Nickel, G.B. Anderson, N.M. Johnson and J. Walker 212

Hydrogen interactions with intrinsic defects in silicon
J.L. Hastings, M. Gharaibeh, S.K. Estreicher and P.A. Fedders 216

Optical absorption study of Zn–H complexes in Si
R. Mori and M. Suezawa 220

Thermal properties of H-related complexes in electron-irradiated Si doped with H
M. Suezawa 224

Hydrogenation and passivation of electron-beam-induced defects in N-type Si
Y. Ohmura, K. Takahashi, H. Saitoh, T. Kon and A. Enosawa 228

Stability and vibrational modes of H_2 and H_2^* complexes in Si
Y.-S. Kim, Y.-G. Jin, J.-W. Jeong and K.J. Chang 231

Hydrogen interaction with defects in electron-irradiated silicon
O. Feklisova, N. Yarykin, Eu. Yakimov and J. Weber 235

Atomic and electronic structure of hydrogen-passivated double selenium donors in silicon
P.T. Huy, C.A.J. Ammerlaan and T. Gregorkiewicz 239

Hydrogen reactions with electron irradiation damage in silicon
A.R. Peaker, J.H. Evans-Freeman, P.Y.Y. Kan, L. Rubaldo, I.D. Hawkins, K.D. Vernon-Parry and L. Dobaczewski 243

Optical absorption due to H-point defect complexes in quenched Si doped with C
N. Fukata and M. Suezawa 247

3.2. Doping and impurities

Breaking through the electrical saturation barrier: 2D- versus 3D-doping in n-type silicon
P.H. Citrin, D. Muller, H.-J. Gossmann, R. Vanfleet and P.A. Northrup 251

Infrared absorption study of a new dicarbon center in silicon
E.V. Lavrov, B.B. Nielsen, J. Byberg and J.L. Lindström 256

A unified microscopic mechanism for donor deactivation in Si
R. Baierle, M.J. Caldas, J. Dąbrowski, H.-J. Müssig and V. Zavodinsky 260

EPR proof of the negatively charged acceptor state Zn^- in silicon
W. Gehlhoff, A. Näser and H. Bracht 264

Theoretical studies of interstitial boron defects in silicon
M. Hakala, M.J. Puska and R.M. Nieminen 268

Defects incorporating Ge atoms in irradiated Si : Ge
N.A. Sobolev and M.H. Nazaré 271

Local vibrational modes of a dicarbon–hydrogen center in crystalline silicon
L. Hoffmann, E.V. Lavrov, B.B. Nielsen and J.L. Lindström 275

Identification of cadmium-related centers in silicon
A. Näser, W. Gehlhoff and H. Overhof 279

Annealing kinetics of the di-carbon radiation-damage centre in edge-defined film-fed growth silicon
S.-C. Park and G. Davies 283

Electron irradiation of heavily doped silicon: group-III impurity ion pairs
V.V. Emtsev, P. Ehrhart, D.S. Poloskin and U. Dedek 287

3.3. Oxygen

Vibrational absorption from vacancy-oxygen-related complexes (VO, V_2O, VO_2) in irradiated silicon
J.L. Lindström, L.I. Murin, V.P. Markevich, T. Hallberg and B.G. Svensson 291

Assignment of EPR spectrum for bistable thermal donors in silicon
L.F. Makarenko, N.M. Lapchuk and Ya.I. Latushko 296

Local vibrational mode bands of V–O–H complexes in silicon
V.P. Markevich, L.I. Murin, M. Suezawa, J.L. Lindström, J. Coutinho, R. Jones, P.R. Briddon and S. Öberg 300

Oxygen and peculiarities of its precipitation in $Si_{1-x}Ge_x$
L.I. Khirunenko, Yu.V. Pomozov, M.G. Sosnin, N.V. Abrosimov, M. Höhne and W. Shröder 305

Oxygen precipitation in nitrogen-doped Czochralski silicon
D. Yang, X. Ma, R. Fan, J. Zhang, L. Li and D. Que 308

An infrared investigation of the 887 cm^{-1} band in Cz–Si
L.G. Fytros, G.J. Georgiou, C.A. Londos and V.V. Emtsev 312

Oxygen in silicon doped with isovalent impurities
L.I. Khirunenko, Yu.V. Pomozov, M.G. Sosnin and V.K. Shinkarenko 317

3.4. Erbium

The temperature dependence of radiative and nonradiative processes at Er–O centers in Si
T.D. Chen, M. Platero, M. Opher-Lipson, J. Palm, J. Michel and L.C. Kimerling 322

Spectroscopic probing of defect-related energy storage in silicon doped with erbium
D.T.X. Thao, T. Gregorkiewicz and J.M. Langer 326

On the generation of optically active Er centers in Si light emitting diodes
W. Jantsch, S. Lanzerstorfer, L. Palmetshofer, M. Stepikhova, G. Kocher and H. Preier 330

Effective Auger excitation of erbium luminescence by hot electrons in silicon
M.S. Bresler, T. Gregorkiewicz, O.B. Gusev, P.E. Pak and I.N. Yassievich 334

The photoluminescence mechanism of erbium in silicon: intensity dependence on excitation power and temperature
D.T.X. Thao, C.A.J. Ammerlaan and T. Gregorkiewicz 338

Er–O clustering and its influence on the lattice sites of Er in Si
U. Wahl, J.G. Correia, J.P. Araújo, A. Vantomme and G. Langouche 342

Impurity effects in silicon implanted with rare-earth ions
V.V. Emtsev, V.V. Emtsev Jr., D.S. Poloskin, E.I. Shek, N.A. Sobolev, J. Michel and L.C. Kimerling 346

Structure of Er-related centers in Si
J.D. Carey and F. Priolo 350

Mechanism of excitation of erbium electroluminescence in amorphous silicon
M.S. Bresler, W. Fuhs, T. Gregorkiewicz, O.B. Gusev, P.E. Pak, E.I. Terukov, K.D. Tsendin and I.N. Yassievich 354

3.5. Metallic impurities

Transition metal defect behavior and Si density of states in the processing temperature regime
A.L. Smith, S.T. Dunham and L.C. Kimerling 358

The electronic configuration of substitutional Fe in silicon
G. Weyer, A. Burchard, M. Fanciulli, V.N. Fedoseyev, H.P. Gunnlaugsson, V.I. Mishin, R. Sielemann and ISOLDE Collaboration 363

Lattice location of implanted Cu in Si
U. Wahl, J.G. Correia, A. Vantomme and G. Langouche 367

Metal impurity precipitates in silicon: chemical state and stability
S.A. McHugo, A.C. Thompson, G. Lamble, C. Flink and E.R. Weber 371

Evidence for deep recombination centers in high-purity silicon from photoluminescence measurements at elevated temperatures
V. Alex and J. Weber 375

Lithium–gold-related complexes in p-type crystalline silicon
J.T. Gudmundsson, H.G. Svavarsson and H.P. Gislason 379

Lattice defects in silicon rapidly solidified from the melt
H. Nishizawa, F. Hori and R. Oshima 383

Copper–hydrogen complexes in silicon
S. Knack, J. Weber and H. Lemke 387

Dissociative diffusion of nickel in silicon, and sinks and sources of vacancy annihilation and generation in the crystal bulk
H. Kitagawa and S. Tanaka 391

Drift of interstitial iron in a space charge region of p-type Si Schottky diode
S. Koveshnikov, B. Choi, N. Yarykin and G. Rozgonyi 395

Impact of vacancies and self-interstitials on the formation of substitutional transition metal defects in float-zone silicon crystals
H. Lemke and W. Zulehner 398

Dependence of electrically detected magnetic resonance signal shape from iron-contaminated silicon wafers on the thermal treatment of the samples
T. Mchedlidze, K. Matsumoto, T.-C. Lin and M. Suezawa 404

Out-diffusion profiles of supersaturated substitutional gold in silicon
M. Morooka 408

What do we know about iron in silicon after 45 yr of research
A.A. Istratov, H. Hieslmair and E.R. Weber 412

Iron-related defect model in n-type silicon based on the electrical and diffusion properties
H. Kitagawa and S. Tanaka 416

The 777 meV photoluminescence band in Si : Pt
J.P. Leitão, M.C. Carmo, M.O. Henry, E. McGlynn, J. Bolmann and S. Lindner 420

Copper-related defects in silicon
S.K. Estreicher 424

Depth profiles of palladium–hydrogen complexes in silicon
J. Weber, S. Knack and J.-U. Sachse 429

Deep level anomalies in silicon doped with radioactive Au atoms
J. Bollmann, S. Lindner, M.O. Henry, E. McGlynn, S. Knack and ISOLDE Collaboration 433

Formation of copper precipitates in silicon
C. Flink, H. Feick, S.A. McHugo, A. Mohammed, W. Seifert, H. Hieslmair, T. Heiser, A.A. Istratov and E.R. Weber 437

Experiments and computer simulations of iron profiles in p/p^+ silicon: segregation and the position of the iron donor level
H. Hieslmair, A.A. Istratov, C. Flink, S.A. McHugo and E.R. Weber 441

ESR study of Fe–H complexes in Si
T. Takahashi and M. Suezawa 445

Pt and Li complexes in silicon. 99-07-22 16.52
M. Kleverman, X. Zhang and J. Olajos 449

3.6. Point and extended defects

A combined experimental and theoretical approach to grain boundary structure and segregation
S.J. Pennycook, M.F. Chisholm, Y. Yan, G. Duscher and S.T. Pantelides 453

Native defects and their interactions in silicon
L. Colombo 458

The structure of vacancy–impurity complexes in highly n-type Si
K. Saarinen, J. Nissilä, H. Kauppinen, M. Hakala, M.J. Puska, P. Hautojärvi and C. Corbel 463

Defect states at silicon surfaces
A.J. Reddy, J.V. Chan, T.A. Burr, R. Mo, C.P. Wade, C.E.D. Chidsey, J. Michel and L.C. Kimerling 468

Effects of extended defects on the properties of intrinsic and extrinsic point defects in silicon
J.F. Justo, A. Antonelli, T.M. Schmidt and A. Fazzio 473

Electron irradiation effects in Si observed at 4.2–25 K by means of in situ transmission electron microscopy
S. Takeda, J. Yamasaki and Y. Kimura 476

Positron annihilation study of dopant effects on proton-irradiation defect in silicon
F. Hori, T. Chijiiwa, R. Oshima and T. Hisamatsu 480

In-situ studies of point-defect complexes in silicon implanted with heavy MeV ions
N. Yarykin, C.R. Cho, R. Zuhr and G. Rozgonyi 485

Impurity-assisted annealing of point defect complexes in ion-implanted silicon
P. Pellegrino, A.Yu Kuznetsov and B.G. Svensson 489

Concentration of point defects in growing CZ silicon crystal under the internal stresses: effects of impurity doping and thermal stress
K. Tanahashi, M. Kikuchi, T. Higashino, N. Inoue and Y. Mizokawa 493

Annealing of the photoluminescence W-center in proton-irradiated silicon
H. Feick and E.R. Weber 497

Magic number vacancy aggregates in Si and GaAs – structure and positron lifetime studies
T.E.M. Staab, M. Haugk, A. Sieck, Th. Frauenheim and H.S. Leipner 501

Interstitial aggregates and a new model for the I_1/W optical centre in silicon
B.J. Coomer, J.P. Goss, R. Jones, S. Öberg and P.R. Briddon 505

Thermal equilibrium concentrations and diffusivities of intrinsic point defects in silicon
T. Okino and T. Shimozaki 509

Nonequilibrium experiments on self-diffusion in silicon at low temperatures using isotopically enriched structures
A. Ural, P.B. Griffin and J.D. Plummer 512

Magic numbers of multivacancy in silicon and its hydrogen decoration
T. Akiyama and A. Oshiyama 516

The divacancy in silicon and diamond
B.J. Coomer, A. Resende, J.P. Goss, R. Jones, S. Öberg and P.R. Briddon 520

Tin-vacancy complexes in e-irradiated n-type silicon
M. Fanciulli and J.R. Byberg 524

3.7. Defects reactions

Effect of high-temperature electron irradiation on the formation of radiative defects in silicon
I.A. Buyanova, T. Hallberg, L.I. Murin, V.P. Markevich, B. Monemar and J.L. Lindström 528

Molecular-dynamics studies of self-interstitial aggregates in Si
M. Gharaibeh, S.K. Estreicher and P.A. Fedders 532

On the fluence dependence of radiation-induced carrier removal in moderately doped Si
H. Amekura, K. Kono and N. Kishimoto 535

Investigation of defect formation and electronic transport in microcrystalline silicon deposited by hot-wire CVD
M. Stöger, A. Breymesser, V. Schlosser, M. Ramadori, V. Plunger, D. Peiró, C. Voz, J. Bertomeu, M. Nelhiebel, P. Schattschneider and J. Andreu 540

Electronic transport properties of polycrystalline silicon films deposited on ceramic substrates
S. Bourdais, G. Beaucarne, J. Poortmans and A. Slaoui 544

Defect diagnostics using scanning photoluminescence in multicrystalline silicon
I. Tarasov, S. Ostapenko, V. Feifer, S. McHugo, S.V. Koveshnikov, J. Weber, C. Haessler and E.-U. Reisner 549

Effects of nitrogen on dislocations in silicon during heat treatment
D. Li, D. Yang and D. Que 553

4. Germanium

Infrared vibrational mode absorption from thermal donors in germanium
P. Clauws and P. Vanmeerbeek 557

Low-temperature spreading-resistance profiling for the characterization of impurity distributions in germanium
S. Voss, H. Bracht and N.A. Stolwijk 561

Frenkel pairs, vacancies, and self-interstitials in Ge: identification and properties from PAC- and Moessbauer spectroscopy
R. Sielemann, H. Haesslein, L. Wende and Ch. Zistl 565

Local vibrational mode spectroscopy of thermal donors in germanium
V.P. Markevich, L.I. Murin, V.V. Litvinov, A.A. Kletchko and J.L. Lindström 570

Electronic and structural properties of vacancy and self-interstitial defects in germanium
A. Janotti, R. Baierle, A.J.R. da Silva, R. Mota and A. Fazzio 575

Investigation of ion-bombardment effects on the formation of voids during deposition of a-Ge : H
Z.L. Peng, D. Comedi, F. Dondeo, I. Chambouleyron, P.J. Simpson and P. Mascher 579

Deep defects in n-type high-purity germanium: quantification of optical variants of deep level transient spectroscopy
A. Blondeel and P. Clauws 584

Initial stages of Ge growth on Si(1 0 0): ad-atoms, ad-dimers, and ad-trimers
G.M. Dalpian, A. Janotti, A. Fazzio and A.J.R. da Silva 589

5. SiGe alloys

Atomic resolution EELS analysis of a misfit dislocation at a GeSi/Si interface
P.E. Batson 593

Diffusion of gold in relaxed Si–Ge epi-layers
R. Fischer, W.F. Frank and K. Lyutovich 598

Deep state defects in strained and relaxed epitaxial $Si_{1-x}Ge_x$ on Si introduced by 3d transition metal and 5d noble metal impurities
K. Nauka and T.I. Kamins 603

Images of local tilted regions in strain-relaxed SiGe layers
P.M. Mooney, J.L. Jordan-Sweet, I.C. Noyan, S.K. Kaldor and P.-C. Wang 608

Growth and dislocation behavior in GeSi bulk alloys
I. Yonenaga 612

Modelling of local modes in Si_xGe_{1-x} and $C_xSi_yGe_{1-x-y}$ alloys to explore the local clustering of the species
S. Scarle and A. Mainwood 616

Site preference next to germanium atom of gold and platinum impurities in SiGe alloy
L. Dobaczewski, K. Bonde Nielsen, K. Gościński, A.R. Peaker and A. Nylandsted Larsen 620

6. Diamond

Jahn–Teller splitting and Zeeman effect of acceptors in diamond
H. Kim, S. Rodriguez, M. Grimsditch, T.R. Anthony and A.K. Ramdas 624

Electron paramagnetic resonance (EPR) and optical absorption studies of defects created in diamond by electron irradiation damage at 100 and 350 K
D.J. Twitchen, D.C. Hunt, M.E. Newton, J.M. Baker, T.R. Anthony and W.F. Banholzer 628

Ab initio calculations of hyperfine interactions for vacancy and Ni point defects in diamond
U. Gerstmann, M. Amkreutz and H. Overhof 632

An orthorhombic nickel–nitrogen complex in high-pressure synthetic diamond
A.J. Neves, M.H. Nazaré, J.C. Lopes and H. Kanda 636

Spin–orbit splitting of acceptor states in Si and C
J. Serrano, A. Wysmolek, T. Ruf and M. Cardona 640

The production and annealing stages of the self-interstitial (R2) defect in diamond
D.J. Twitchen, D.C. Hunt, C. Wade, M.E. Newton, J.M. Baker, T.R. Anthony and W.F. Banholzer 644

Transition metals in diamond: experimental and theoretical identification of Co–N complexes
K. Johnston, A. Mainwood, A.T. Collins, G. Davies, D. Twitchen, J.M. Baker and M. Newton 647

New paramagnetic defects in synthetic diamonds grown using nickel catalyst
A.J. Neves, R. Pereira, N.A. Sobolev, M.H. Nazaré, W. Gehlhoff, A. Näser and H. Kanda 651

7. Silicon carbide

Electron-paramagnetic-resonance studies of defects in electron-irradiated p-type 4H and 6H SiC
N.T. Son, P.N. Hai, P.T. Huy, T. Gregorkiewicz, C.A.J. Ammerlaan, J.L. Lindström, W.M. Chen, B. Monemar and E. Janzén 655

Effective mass donors in silicon carbide — a study with electron nuclear double resonance
S. Greulich-Weber, M. März and J.-M. Spaeth 659

Zeeman spectroscopy of the neutral silicon vacancy in 6H and 4H SiC
Mt. Wagner, B. Magnusson, E. Sörman, C. Hallin, J.L. Lindström, W.M. Chen and E. Janzén 663

Electron paramagnetic resonance of the scandium acceptor in 4H and 6H silicon carbide
J.-M. Spaeth, S. Greulich-Weber, M. März, E.N. Mokhov and E.N. Kalabukhova 667

Low-dose ion implanted epitaxial 4H–SiC investigated by deep level transient spectroscopy
D. Åberg, A. Hallén and B.G. Svensson 672

Zeeman spectroscopy of the D_1 bound exciton in 3C–, and 4H–SiC
T. Egilsson, I.G. Ivanov, A. Henry and E. Janzén 677

Effect of grown-in biaxial strain on deep level defects in $Si_{1-y}C_y$/Si epitaxial heterostructures
D.V. Singh, T.O. Mitchell, J.L. Hoyt, J.F. Gibbons, N.M. Johnson and W.K. Götz 681

8. GaAs and AlGaAs

8.1. Point and extended defects

Self-diffusion on the arsenic sublattice in GaAs investigated by the broadening of buried nitrogen doping layers
N.A. Stolwijk, G. Bösker, J.V. Thordson, U. Södervall, T.G. Andersson, Ch. Jäger and W. Jäger 685

Hydrogen passivation of $Al_xGa_{1-x}As$/GaAs studied by surface photovoltage spectroscopy
H.Ö. Olafsson, J.T. Gudmundsson, H.G. Svavarsson and H.P. Gislason 689

Deep-level defects near the surface of Be-doped GaAs grown by molecular beam epitaxy
P. Krispin, M. Asghar, H. Kostial and R. Hey 693

Diffusivity of arsenic interstitials in GaAs studied by sulfur in-diffusion
H.S. Leipner, R.F. Scholz, N. Engler, F. Börner, P. Werner and U. Gösele 697

Effect of lithium diffusion on the native defects in GaAs studied by positron annihilation spectroscopy
S. Arpiainen, K. Saarinen, J.T. Gudmundsson and H.P. Gislason 701

Influence of stoichiometry and doping on vacancies in n-type GaAs
J. Gebauer, M. Lausmann, F. Redmann and R. Krause-Rehberg 705

Defect investigations in plastically deformed gallium arsenide
H.S. Leipner, C.G. Hübner, P. Grau and R. Krause-Rehberg 710

Formation of vacancy clusters during copper diffusion in GaAs
R. Krause-Rehberg, K. Petters and J. Gebauer 714

Deep levels in He^{++} irradiated Be-doped $Al_{0.5}Ga_{0.5}As$ MBE layers
J. Szatkowski, E. Placzek-Popko, K. Sieranski, O.P. Hansen, A. Johansen and C. Soerensen 718

Native point defect analysis in non-stoichiometric GaAs: an annealing study
R.C. Lutz, P. Specht, R. Zhao, O.H. Lam, F. Börner, J. Gebauer, R. Krause-Rehberg and E.R. Weber 722

As antisite incorporation in epitaxial growth of GaAs
J.C. Bourgoin, H. Hammadi, M. Stellmacher, J. Nagle, B. Grandidier, D. Stievenard, J.P. Nys, C. Delerue and M. Lannoo 725

Extrinsic and intrinsic defects at molecular-beam-epitaxy regrown GaAs interfaces
N.H. Ky, D. Martin and F.K. Reinhart 729

Femtosecond nonlinear optics of low-temperature grown semiconductors
U. Siegner, M. Haiml, F. Morier-Genoud, R.C. Lutz, P. Specht, E.R. Weber and U. Keller 733

8.2. Impurities

Tunnel ionization of deep impurities in semiconductors induced by terahertz electric fields
S.D. Ganichev 737

Hydrogen molecules in GaAs after hydrogen plasma treatment
A.W.R. Leitch and J. Weber 743

Photo-ionization spectra for alloy-induced configurations of Si–DX center in AlGaAs
R. Piotrzkowski 746

Photoluminescence of highly compensated GaAs doped with high concentration of Ge
M. Watanabe, A. Watanabe and M. Suezawa 750

Reactions of column-III vacancies and interstitials during Zn diffusion-induced disordering of GaAs/AlGaAs multiple-quantum-well structures
N.H. Ky 754

Ab initio calculation of local vibrational modes. Application to GaAs:C and cubic GaN:As
C. Göbel, K. Petzke, C. Schrepel and U. Scherz 759

Dopant-related metastable defects in particle irradiated n-GaAs
M.J. Legodi, F.D. Auret and S.A. Goodman 762

Terahertz tunnel ionization of DX-centers in AlGaAs : Te
H. Ketterl, E. Ziemann, S.D. Ganichev, I.N. Yassievich, A. Belyaev, S. Schmult and W. Prettl 766

Luminescence properties of Er,O-codoped III–V semiconductors grown by organometallic vapor phase epitaxy
Y. Fujiwara, T. Kawamoto, T. Koide and Y. Takeda 770

Direct observation of local structure of DX center by capacitance X-ray absorption fine structure
M. Ishii, Y. Yoshino, K.-i. Takarabe and O. Shimomura 774

Influence of oxygen co-doping on the thermal quenching property of Er-related emission in $Al_{0.70}Ga_{0.30}As$: Er
S. Uekusa, K. Uchiya and M. Kumagai 778

Optical ionization of DX center in AlGaAs : Se by inner-shell excitation
Y. Yoshino, K. Takarabe, M. Ishii, Y. Katayama and O. Shimomura 781

Mechanism for dicarbon defect formation in AlAs and GaAs
C.D. Latham, R. Jones, M. Haugk, Th. Frauenheim and P.R. Briddon 784

Vibrational excited-state transitions of substitutional carbon in gallium arsenide
H.Ch. Alt 788

New type of persistent photoconductivity related to DX-center: the study of interband PPC in Si-doped AlGaAs
R. Piotrzkowski, E. Litwin-Staszewska, F. Bosc, J. Sicart and J.L. Robert 792

9. Other III–V compounds

Comparison of electronic and mechanical contrast in scanning tunneling microscopy images of semiconductor heterojunctions
R.M. Feenstra 796

Complexes of group-VI donors with hydrogen in GaP
B. Clerjaud, D. Côte and W. Ulrici 803

Local-vibrational-mode absorption of interstitial oxygen in GaP
W. Ulrici, B. Clerjaud and D. Côte 807

Optical and magnetic resonance studies of As-impurities in AlSb: from isoelectronic point defects to planes
E.R. Glaser, T.A. Kennedy, B.R. Bennett, B.V. Shanabrook, L.A. Hemstreet, M.W. Bayerl and M.S. Brandt 811

Deep electronic states near the surface of (In,Ga)P layers grown by MOVPE on GaAs
P. Krispin, M. Asghar and A. Knauer 815

Interplay between Jahn–Teller coupling and axial crystal fields: GaP:(Cr, S)
E. Baars, A. Dörnen and W. Ulrici 819

Modeling the diffusion of Be in InGaAs/InGaAsP epitaxial heterostructures under non-equilibrium point defect conditions
K. Ketata, M. Ketata, S. Koumetz, J. Marcon and O. Valet 823

Local vibrational modes associated with semi-insulating InP : C, frequencies and line shapes
R.C. Newman, B.R. Davidson, R.S. Leigh, M.J.L. Sangster and C.C. Button 827

Intrinsic doping in InP: ab initio calculations of P_{In} antisites
T.M. Schmidt, R.H. Miwa, A. Fazzio and R. Mota 831

Structural and electronic properties of doped InP/InGaAs short period superlattices grown by LP-MOVPE
A.B. Henriques, L.K. Hanamoto, R.F. Oliveira, P.L. Souza, L.C.D. Gonçalves and B. Yavich 835

Deep levels associated with alpha irradiation of n-type MOCVD InP
M.Z. Iqbal, U.S. Qurashi, A. Majid, A. Khan, N. Zafar, A. Dadgar and D. Bimberg 839

10. II–VI compounds

Defect complexes induced by diffusion of group I acceptors into CdTe
H. Wolf, T. Filz, J. Hamann, S. Lany, V. Ostheimer and Th. Wichert 843

Intra-shell transitions of 3D metal ions (Fe, Co, Ni) in II–VI wide-gap semiconductor alloys
T.P. Surkova, M. Godlewski, K. Swiatek, P. Kaczor, A. Polimeni, L. Eaves and W. Giriat 848

NMR study of bistable defects under in situ illumination
M. Shroyer, J.K. Furdyna, A.I. Ryskin and W.W. Warren Jr. 852

Shallow doping of wide band-gap II–VI compounds
B. Reinhold and M. Wienecke 856

The electronic structure of interstitial zinc in its two T_d sites in ZnSe
K.H. Chow and G.D. Watkins 861

Ab initio study of local vibrational modes in II–VI semiconductors: ZnS:Se and ZnSe:N
K. Petzke 866

Luminescence and influence of defect concentration on excitons in $^{197}Hg/^{197}Au$-doped CdTe
J. Hamann, A. Burchard, M. Deicher, T. Filz, V. Ostheimer, F. Strasser, H. Wolf, ISOLDE Collaboration and Th. Wichert 870

Lattice site and diffusion of ion-implanted Li in as-grown and Se-rich ZnSe
K. Bharuth-Ram, M. Restle, H. Hofsäss, C. Ronning and U. Wahl 875

Persistent photoconductivity and DLTS in indium-doped $Cd_{0.9}Mn_{0.1}Te$
J. Szatkowski, E. Placzek-Popko, K. Sierański, J. Fialkowski, J.M. Wrobel and P. Becla 879

Photoluminescence of deep levels in (CdZn) Te-correlation with diffusion length measurement
J. Franc, P. Hlídek, H. Sitter, E. Belas, A.L. Toth, L. Turjanska and P. Höschl 883

Study of microscopic mechanisms of electrical compensation of donors in CdS by fast diffusors (Cu, Ag, or Au)
I.D. Desnica-Frankovic, U.V. Desnica, A. Stötzler and M. Deicher 887

Hydrogen passivation of nitrogen-related energy levels in ZnSe and ZnSSe grown by MBE
D. Seghier, J.T. Gudmundsson and H.P. Gislason 891

Anisotropic polarization of dislocation-related luminescence in thin ZnSe films
L. Worschech, W. Ossau, A. Waag, G. Landwehr, U. Hilpert, J. Schreiber, Y.T. Rebane and Y.G. Shreter 895

Induced defects in ZnS by electron and proton irradiation and defect-annealing behavior
S. Brunner, W. Puff, A.G. Balogh and P. Mascher 898

The deactivation of nitrogen acceptors in ZnS_xSe_{1-x} and $Mg_yZn_{1-y}S_xSe_{1-x}$ studied by combining positron annihilation, SIMS, and CV measurements
J. Oila, K. Saarinen, T. Laine, P. Hautojärvi, P. Uusimaa, M. Pessa and J. Likonen 902

Compensating defects and electrical activation of donors in CdS
U.V. Desnica, I.D. Desnica-Frankovic, R. Magerle and M. Deicher 907

Spin-flip Raman scattering in submonolayer CdSe/ZnSe structures
T. Ruf, O.Z. Karimov, D. Wolverson, J.J. Davies, A.N. Reznitsky, A.A. Klochikhin, S.Yu. Verbin, L.N. Tenishev, S.A. Permogorov and S.V. Ivanov 911

11. Other semiconductors

Evidence on a bond-breaking relaxation in the bistable centers In and Ga in CdF_2
J. Nissilä, K. Saarinen, P. Hautojärvi, A. Suchocki and J.M. Langer 915

Analysis of secondary phases in InSbBi thin films
M.C. Wagener, R.E. Kroon, J.R. Botha and A.W.R. Leitch 919

Determination of deep and shallow levels in conjugated polymers by electrical methods
P. Stallinga, H.L. Gomes, H. Rost, A.B. Holmes, M.G. Harrison, R.H. Friend, F. Biscarini, C. Taliani, G.W. Jones and D.M. Taylor 923

Differences in the electronic structure and compensation mechanism between n-type Zn- and Cd-doped $CuInS_2$ crystals
T. Yamamoto, I.V. Luck, R. Scheer and H. Katayama-Yoshida 927

Defects in CuIn(Ga)Se_2 solar cell material characterized by positron annihilation: post-growth annealing effects
F. Börner, J. Gebauer, S. Eichler, R. Krause-Rehberg, I. Dirnstorfer, B.K. Meyer and F. Karg 930

Do structural defects affect semiconducting properties of fullerene thin films?
E.A. Katz, A.I. Shames, D. Faiman, S. Shtutina, Y. Cohen, S. Goren, W. Kempinski and L. Piekara-Sady 934

12. Low-dimensional studies

Confinement effects on phosphorus donors embedded in silicon nanocrystals
B.J. Pawlak, T. Gregorkiewicz and C.A.J. Ammerlaan 938

Determination of potential fluctuations in modulation-doped SiGe-quantum wells from conduction electron spin resonance
W. Jantsch, Z. Wilamowski, N. Sandersfeld, F. Schäffler 944

Phonon resonances in optical spectra of donors in quantum wells
S. Bednarek, B. Szafran, J. Adamowski, I. Essaoudi and B. Stébé 947

Boron in mesoporous Si — Where have all the carriers gone?
G. Polisski, D. Kovalev, G. Dollinger, T. Sulima and F. Koch 951

OH-related emitting centers in interface layer of porous silicon
T.V. Torchynska, M.K. Sheinkman, N.E. Korsunskaya, L.Yu. Khomenkovan, B.M. Bulakh, B.R. Dzhumaev, A. Many, Y. Goldstein and E. Savir 955

Hole and electron traps in the InGaAs/GaAs heterostructures with quantum dots
M.M. Sobolev, I.V. Kochnev, V.M. Lantratov, N.A. Cherkashin and V.V. Emtsev 959

Defect-limited carrier diffusion in $In_{0.53}Ga_{0.47}As$-InP single quantum well
A.F.G. Monte, S.W. da Silva, J.M.R. Cruz, P.C. Morais and H.M. Cox 963

Optical and magnetic properties for erbium-related centres in self-assembly silicon nanostructures
N.T. Bagraev, A.D. Bouravleuv, W. Gehlhoff, L.E. Klyachkin, A.M. Malyarenko, M.M. Mezdrogina, A. Naeser, V.V. Romanov and S.A. Rykov 967

Non-exponential capture of electrons in GaAs with embedded InAs quantum dots
C. Walther, J. Bollmann, H. Kissel, H. Kirmse, W. Neumann and W.T. Masselink 971

13. Novel theoretical and experimental approaches

Overcoming doping bottlenecks in semiconductors and wide-gap materials
S.B. Zhang, S.-H. Wei and A. Zunger 976

Diffusion in isotopically controlled semiconductor systems
H. Bracht 981

Calculation of the line shapes of electronic transitions at defects using the frozen Gaussian technique
B. McKinnon, A. Mainwood and A.M. Stoneham 987

First-principles dynamics of defect reactions triggered by electronic excitation
Y. Miyamoto, O. Sugino and Y. Mochizuki 991

Numerical determination of one-dimensional energy bands bound to dislocations
J.L. Farvacque and Ph. François 995

Transient lattice vibration induced by coherent carrier captures at a deep-level defect and the effect on defect reactions
Y. Shinozuka and T. Karatsu 999

Real-space electronic structure calculations of charged clusters and defects in semiconductors using a multigrid method
Y.-G. Jin, J.-W. Jeong and K.J. Chang 1003

Magnetic field effect on tunnel ionization of deep impurities by far-infrared radiation
A.S. Moskalenko, S.D. Ganichev, V.I. Perel and I.N. Yassievich 1007

Study of bound exciton excited state structure using photothermal ionisation spectroscopy
M. Gibson, E. McGlynn and M.O. Henry 1011

14. Defects in devices

Electron spin resonance study of the interaction of hydrogen with the (1 1 1)Si/SiO_2 interface: P_b-hydrogen interaction kinetics
A. Stesmans 1015

Aspects of defects in silica related to dielectric breakdown of gate oxides in MOSFETs
P.E. Blöchl and J.H. Stathis 1022

Capacitively detected magnetic resonance of defects in MOSFETs
M.S. Brandt, R. Neuberger and M. Stutzmann 1027

Radiation-induced lattice defects in InGaAsP laser diodes and their effects on device performance
H. Ohyama, E. Simoen, C. Claeys, T. Hakata, T. Kudou, M. Yoneoka, K. Kobayashi, M. Nahabayashi, Y. Takami and H. Sunaga 1031

Impact of induced lattice defects on performance degradation of AlGaAs/GaAs p-HEMTs
T. Hakata, H. Ohyama, S. Kuroda, E. Simoen, C. Claeys, T. Kudou, K. Kobayashi, M. Nakabayashi, M. Yoneoka, Y. Takami, H. Sunaga and K. Miyahara 1034

Mechanism of injection-enhanced defect transformation in LPE GaAs structures
T.V. Torchynska, G.P. Polupan, V.I. Kooshnirenko and E. Scherbina 1037

The bulk damaged effects of clustered defects in irradiated silicon detectors
S. Saramad and A.M. Zarandi 1041

Defect-engineering rad-hard particle detectors: the role of impurities and inter-defect charge exchange
B.C. MacEvoy, A. Santocchia and G. Hall 1045

Point defect reaction in (Al)GaInP STQW lasers enhanced by laser operation
A. Ihara, Y. Ohno, S. Takeda, S. Nagao, D. Diffily, Y. Satoh, K. Shimoyama and N. Hosoi 1050

List of Contributors 1054

Subject Index 1060